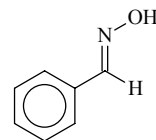
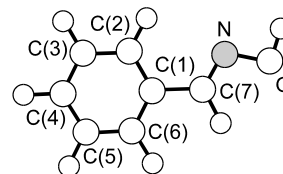


798 **C₇H₇NO**MW, *ab initio*
calculations**(E)-Benzaldehyde oxime****C_s**

r_0 ^{a)}	Å ^{b)}	θ_0 ^{a)}	deg ^{b)}
C(1)–C(2)	1.3997(20)	C(2)–C(1)–C(6)	119.57(20)
C(1)–C(6)	1.4028(30)	C(2)–C(1)–C(7)	121.92(10)
C(1)–C(7)	1.4652(50)	C(6)–C(1)–C(7)	118.51(20)
C(2)–C(3)	1.3942(50)	C(1)–C(2)–C(3)	119.79(10)
C(2)–H	1.0822(30)	C(2)–C(3)–C(4)	120.56(20)
C(3)–C(4)	1.3984(30)	C(3)–C(4)–C(5)	119.72(20)
C(3)–H	1.0833(10)	C(4)–C(5)–C(6)	119.93(10)
C(4)–C(5)	1.3959(20)	C(1)–C(6)–C(5)	120.42(20)
C(4)–H	1.0824(40)	C(1)–C(7)–N	120.69(20)
C(5)–C(6)	1.3939(50)	C(7)–N–O	109.88(20)
C(5)–H	1.0829(20)	C(1)–C(2)–H	119.39(20)
C(6)–H	1.0845(10)	C(2)–C(3)–H	119.56(10)
C(7)–N	1.2908(30)	C(3)–C(4)–H	120.10(20)
C(7)–H	1.0895(10)	C(4)–C(5)–H	120.22(20)
N–O	1.4094(40)	C(5)–C(6)–H	120.09(10)
O–H	0.9663(20)	N–C(7)–H	120.07(20)
		N–O–H	101.72(20)

The molecular conformation is planar. The CCNO and CNOH dihedral angles are both nearly equal to 180°; *i.e.*, the conformations of the two groups are both close to *anti*.



^{a)} *Ab initio* (MP2/6-31G(d,p)) geometry was scaled so as to reproduce the observed rotational constants.

^{b)} Uncertainties are ten times those of the original paper.

Kuze, N., Sato, M., Maue, K., Usami, T., Sakaizumi, T., Ohashi, O., Iijima, K.: J. Mol. Spectrosc. **196** (1999) 283.